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ANGULAR MOTION OF A PAH MOLECULE IN INTERSTELLAR ENVIRONMENT

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The Polycyclic Aromatic Hydrocarbon (PAH) molecules have recently been proposed as an important and hitherto undetected component of the ISM. The hypothesis was based on an attractive explanation of the "Unidentified IR Emission Bands" (Léger and Puget 1984). It has already led to a verified prediction on extended galactic and extragalactic emissions measured by IRAS (Boulanger et al., 1986), or by a recent balloon-borne experiment (Giard et al., 1988). We study here the physics that rules the motion of such molecules in the ISM, taking into account their coupling with the ambient gas, the radiation field (absorption and emission) and the static magnetic field. This study is important for many implications of the PAH hypothesis such as the radio emission by these molecules or the expected polarization of their IR emission (Sellgren et al., 1988).

We consider a reflection nebulae where the situation is rather well known (Omont, 1986). Every day life of a mean PAH molecule in such a region is as follows: every three hours a UV photon is absorbed heating the molecule to a thousand degree; the temperature decay due to cooling by infrared emission follows then within a few seconds. A collision with a molecule of gas occurs typically once every week, while an H atom is ejected or captured at the same rate. The figure 1 gives a typical cooling cycle after a heat impulse.

The PAH molecule we have considered as representative of the family has typically 50 atoms, a radius of 4.5 Å, is circular and has a molecular mass $M = 300$; its permanent dipole moment is 3 Debye.

The four basic questions we try to answer are: *i)* what are the interactions that make the molecule rotating; what is the rotational velocity or more precisely the statistical distribution $n(J)$ of the angular momentum \vec{J} ; *ii)* does the molecule rotate preferentially around an axis normal to its plane ? or more precisely what is the distribution $n(K)$ of the projection of \vec{J} on the main axis of inertia; *iii)* is alignment possible, either on the magnetic field or on the line of sight of a source of photons through *streaming* process ? *iv)* finally what are the implications in terms of observations of the rotation of PAHs ?

Rotational velocity: The distribution $n(J)$ results from a random walk where the different events giving rise to a variation of J are a collisions, the accretion or the ejection of a H atom, the emission or the absorption of a photon (UV, IR or radio). Rotational drag from the interstellar gas, radio emission of rotational photons or self-regulating disymmetry of the probabilities of IR photo-emission will limit the growth of the rotational velocity.

PAHs eject H-atoms by thermo-dissociation; this uses a fraction of a vibration quanta (.04 eV) and produces suprathermal H-atoms (900K). Photo-dissociation is another possible mechanism (Buch, 1988), however not yet proven in large molecules, much more efficient (2.5 eV and 30 000K). When absorbing or emitting a photon, the angular momentum exchange is $\Delta J = 0, \pm 1$. The absorption of one UV photon is followed by the emission of a burst of typically 50 IR photons.

We give in table I the different contributions of each process to the random-walk building-up and to its limitation by drag type effects.

Physical process	Rate	ΔJ (random)	δJ (drag)
Collision with a H atom	once a week	$\pm 10 \hbar$	$-J/150$
Ejection of a H atom (thermo-dissociation)	once a week	$\pm 6 \hbar$	$-J/100$
Emission of an IR photon (vibr-rot)	50 each 3 hours	$\pm \hbar$	$-\frac{[J - \langle J \rangle]}{3000}$
Emission of a radio photon (rot)	one photon per day		$-\hbar$

All these contributions can be handled through a Focker-Planck equation describing the global diffusion-like process.

We have shown that the dominant mechanism in the building-up of J is either photo-dissociation, if real, with $\langle J \rangle = 220$ and $T_{rot} = 760K$, or IR emission which leads typically to $\langle J \rangle = 80 \pm 70$ and $T_{rot} = 130K$. *Radio emission is in both cases very efficient.* The figure 2 displays the distribution of J for the second case, the most likely. One shows that this distribution is thermal with a temperature $T_{rot} = \frac{h\nu_0}{6}$, where ν_0 is the -properly averaged- frequency of IR vibration-rotation photons.

Alignment of \vec{J} perpendicular to the molecule plane: The distribution $n(K)$ results from internal energy exchange with the vibration modes of the molecule, allowing the conservation of \vec{J} and total energy $E = E_{rot} + E_{vib}$. This Intramolecular Vibration-Rotation Energy Transfert (IVRET) is caused by Coriolis and centrifugal interactions. As \vec{J} is fixed, the change in E_{rot} must be the result of a change in K , thus affecting the precession angle (β) the symmetry axis makes with \vec{J} . This angle changes many times during each UV photon event and K is statistically distributed with the vibrational temperature T_{vib} at each moment. When the rotational temperature T_J which characterizes J is much higher than T_K , the molecule axis aligns along \vec{J} ($K \rightarrow J$); when $T_J \ll T_K$, the axis is isotropically distributed around \vec{J} (uniform distribution of K from: $-J$ to $+J$) :

this happens just after the absorption of a UV photon.

Cooling of the molecule tends thus to a rapid (a few hundred seconds) alignment of the rotation vector normal to the plane, and memory of the direction of the UV photon is thus immediately lost after its absorption.

Streaming: Alignment of non-spherical grains by streaming supposes that a driving force, the radiative pressure, at least equal to the gas pressure times the surface area of the grain maintains a velocity of the particle with respect to the gas (Roche and Aitken 1985). The resulting unbalance of the collision directions tends to favorise a spinning with an axis preferentially oriented perpendicular to the stream. We have shown that the radiative pressure is in general too weak in a typical reflecting nebula to drive a PAH molecule at a velocity significantly different from the thermal velocity: *streaming is thus unefficient*.

Coupling with \vec{B} : The coupling of the molecule with the interstellar magnetic field $\vec{B} = 10\mu\text{Gauss}$ causes its precession around the field direction with a period $\nu_{\text{Larmor}}^{-1} \simeq 3000s$ much larger than the cooling time ($t_{IR} = 3s$). This results from the evaluation of the permanent magnetic moment (μ) of the molecule, considering rotation of a charged system when ionized, diamagnetism, Barnett effect, electronic orbital and spin magnetic moment; the last two ones could be in principle as large as one Bohr magneton (μ_0). However the quenching to zero of the orbital momentum in aromatic molecules reduces $\langle \vec{L} \rangle$ directly and $\langle \vec{S} \rangle$ via the spin-orbit coupling.

A second possible effect of \vec{B} we have investigated is the Davis-Greenstein alignment mechanism proposed for interstellar grains. However the very large imaginary part of the susceptibility it supposes (super ferro-magnetism, Mathis 1986) can hardly be found in PAH molecules, and we do not believe such a mechanism of alignment can be efficient.

Radio emission: because of the rapid rotation one expects a significant radio emission due to transitions between rotational levels. Because the molecule rotates most of the time around its largest axis of inertia, we have used the approximation of linear molecules to evaluate the power radiated by PAHs. The different quantities of interest are given below, and the radio spectrum is displayed on figure 3.

- Spontaneous emission: $A_{J \rightarrow J-1} = 9 \cdot 10^{-12} \left(\frac{\mu}{3Debye} \right)^2 J^3 \text{ s}^{-1}$
- Emission spectrum: $P_\nu \propto \nu^5 \exp\left[-\frac{h^2 \nu^2}{4BkT_{rot}}\right]$
- $\nu_{max} = 87 \left(\frac{N_{at}}{24} \right)^{-\frac{5}{4}} GHz \Rightarrow \lambda_{max} = 3.4 \left(\frac{N_{at}}{24} \right)^{\frac{5}{4}} \text{ mm}$
- Integrated emitted power per molecule:
 $6.5 \cdot 10^{-21} \left(\frac{\mu}{3D} \right)^2 \left(\frac{N_{at}}{24} \right)^{\frac{5}{2}} \text{ erg s}^{-1}$
- Radiated power per h atom:
 $L_H^{PAH} = 4.5 \cdot 10^{-34} \left(\frac{\mu}{3D} \right)^2 \left(\frac{N_{at}}{24} \right)^{\frac{3}{2}} W H_{at}^{-1}$

- Source brightness (for $A_v = 1$):

$$B_{(3mm)}^{PAH} = 1.0 \left(\frac{N_{dust}}{24} \right)^{\frac{3}{2}} MJ_y sr^{-1} mag^{-1}$$

- For comparison:

- Thermal grain emission:

$$B_{(3mm)}^{dust} = .006 MJ_y sr^{-1} mag^{-1}$$

- Average molecular brightness (Galactic Center direction):

$$B_{(3mm)}^{molec} = .2 MJ_y sr^{-1} mag^{-1}$$

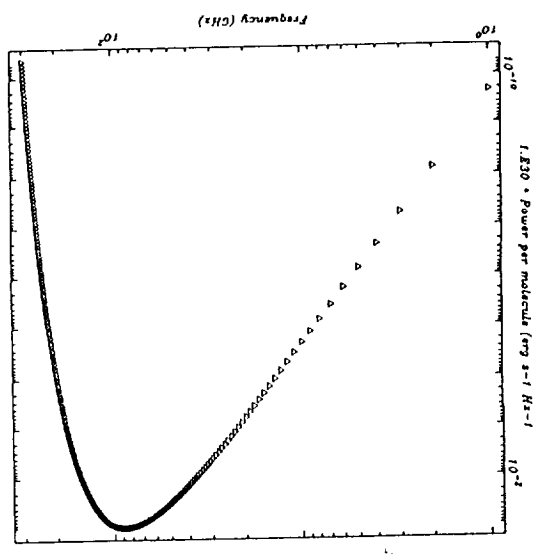
We conclude that *the radio emission of PAH molecules would dominate the millimetric radio continuum from reflecting nebula*. This represents a new observational test of the PAH hypothesis.

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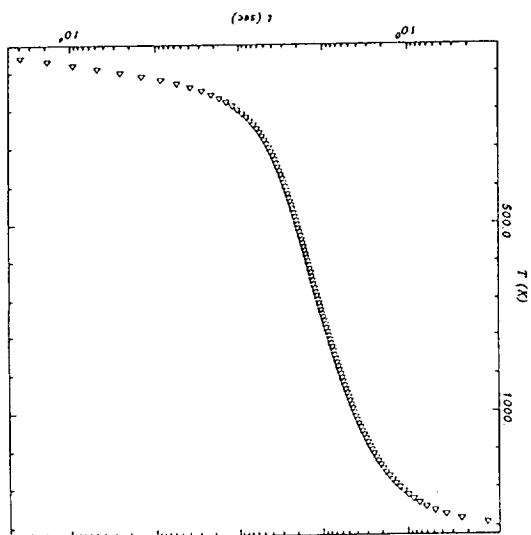
Radio emission spectrum of a
population of PAHs

Figure 3



Cooling of a PAH after a heat impulse

Figure 1



Statistical distribution of the angular momentum number J when governed by the
emission of IR vibration-rotation photons.

Figure 2

